Glutaric acid, di(3-fluorobenzyl) ester

Inchi: InChI=1S/C19H18F2O4/c20-16-6-1-4-14(10-16)12-24-18(22)8-3-9-19(23)25-13-15-5-2-7
InchiKey: MBENIUYCDXYWPV-UHFFFAOYSA-N
Formula: C19H18F2O4
SMILES: O=C(CCCC(=O)OCc1cccc(F)c1)OCc1cccc(F)c1
Mol. weight [g/mol]: 348.34

Physical Properties

Property code	Value	Unit	Source
gf	-542.80	kJ/mol	Joback Method
hf	-867.19	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.922		Crippen Method
mcvol	249.470	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	848.56	K	Joback Method
tc	1062.01	K	Joback Method
tf	527.27	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.08	J/mol×K	848.56	Joback Method
cpg	751.06	J/mol×K	884.14	Joback Method
cpg	762.90	J/mol×K	919.71	Joback Method
cpg	773.64	J/mol×K	955.29	Joback Method
cpg	783.29	J/mol×K	990.86	Joback Method
cpg	791.90	J/mol×K	1026.44	Joback Method
cpg	799.48	J/mol×K	1062.01	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume